

Characterization of stacking faults in 4H-SiC epilayers by room-temperature microphotoluminescence mapping

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The stacking faults (SFs) in 4H-SiC epilayers have been characterized by microphotoluminescence spectroscopy and photoluminescence (PL) intensity mapping at room temperature. Three kinds of SFs, intrinsic Frank SFs, double Shockley SFs, and in-grown SFs, have been identified in the samples. Each kind of SF shows the distinct PL emission located at 420, 500, and 455 nm, respectively. The shapes and distributions of SFs have been profiled by micro-PL intensity mapping. The formation mechanisms of each SF are also discussed. © 2008 American Institute of Physics. [DOI: 10.1063/1.2937097]

Silicon carbide (SiC) is an attractive material for developing high-power, high-temperature, and high-frequency devices, owing to its superior properties.¹ However, the commercialization of 4H-SiC high-voltage *p-i-n* diodes has been hampered by the degradation problem of their forward *I-V* characteristics.^{2,3} This effect is attributed to the formation and expansion of stacking faults (SFs) in the blocking layer.⁴ In order to minimize the deleterious effects of SFs on 4H-SiC device structures, the formation of these SFs must be understood so that an effective approach for controlling them can be formulated. Meanwhile, a highly practical and nondestructive analysis method is imperative for spatial profiling of SFs in SiC wafers and to directly compare the SFs and the device performance.

Several techniques can be utilized to identify the SFs in SiC, such as transmission electron microscopy (TEM), cathodoluminescence, KOH etching, x-ray topography, and microphotoluminescence (micro-PL) mapping. The micro-PL mapping is a nondestructive method which has been used to characterize the dislocations and micropipes in the whole SiC wafer area, and it is very sensitive to the electrically active defects in the material.^{5,6} In recent years, the micro-PL mapping was performed to characterize the replication of SFs from 4H-SiC substrates into epilayers.⁷ However, there is still lack of fundamental data, especially the room-temperature PL spectra from different SFs in 4H-SiC. In this letter, micro-PL measurements have been carried out to characterize the defects, especially SFs, in 4H-SiC epilayers. From room-temperature PL spectra, three kinds of SFs have been identified. The shape, distribution, and possible origins of each SF in the epilayer are discussed based on micro-PL mapping data.

4H-SiC epilayers were grown on 8° off-axis 4H-SiC (0001) *n*⁺ substrates (doping concentration: $(5-6) \times 10^{18} \text{ cm}^{-3}$) by horizontal hot-wall chemical vapor deposition in a SiH₄-C₃H₈-H₂ system.⁸ Epitaxial growth was performed at 1650 °C with a reactor pressure of 80 Torr and the C/Si ratio of 0.9. The growth rate was 12–25 μm/h and the thickness of epilayer was approximately 55 μm. The epilayer

was intentionally doped with the nitrogen donors to $1.5 \times 10^{15} \text{ cm}^{-3}$. Micro-PL spectroscopy and PL intensity mapping were performed on the samples by using a PLMicro-SiC by Nanometrics Inc. PL was excited by the 25 mW, 325 nm line of a He–Cd laser, dispersed with a grating monochromator, and detected by a photomultiplier. The excitation beam was chopped and a lock-in amplifier was used to extract the weak PL signal. The extensive efforts were performed on the optics and detection channels in order to provide enhanced sensitivity in the UV spectral region. The laser beam was focused to a spot with a diameter of about 0.8 μm using a sapphire objective lens. The sample was mounted on the XYZ stage with a spatial resolution of 0.5 μm. The setup can acquire data in a single wavelength mode (PL intensity mapping mode) or in a full spectral scanning mode (PL spectroscopy mode), with the spectral resolution of 1 nm.

Figure 1(a) shows a typical micro-PL spectrum from a 4H-SiC epitaxial layer without SFs at room temperature. The main feature is a 4H band-edge peak at 386 nm with a tail at the low energy side. In general, the intensity of the band-edge emission is decreased by the nonradiative recombination via defect levels and surface/interface recombination. As a result, the intensity variation of band-edge emission reflects the distribution of crystalline quality (or defects) in the sample. Due to the indirect bandgap structure of the SiC crystals, the recombination lifetime in 4H-SiC is relatively long, in the order of a few μs, which was determined by microwave photoconductance decay measurements.⁹ In this case, the diffusion length of the excited carriers can be very long, even several tens of μm, though the penetration depth of the 325 nm laser is only ~8 μm in 4H-SiC.¹⁰ Thus, the crystalline-quality information in the deep region, for example, near the substrate/epilayer interface, can be detected by the current PL configurations. Due to the considerable difference of the carrier lifetime between the epilayer and the substrate (~0.04 μs), however, the information inside the substrate can be hardly observed in the PL spectra. The variation of PL intensity of the band-edge emission peak can be utilized to reflect the distribution of crystalline defects only in the epilayers.

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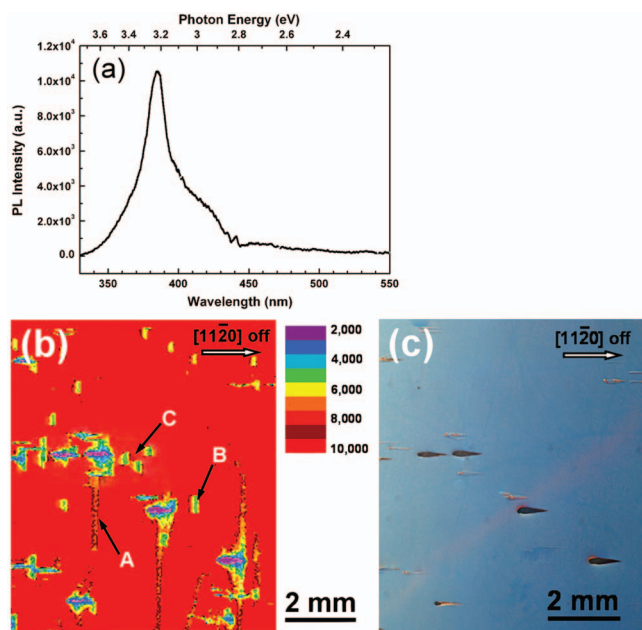


FIG. 1. (Color) (a) Micro-PL spectrum from the 4H-SiC epilayer (without SFs) at room temperature, (b) PL intensity mapping at 386 nm, and (c) optical microscopy image of the sample surface.

Figure 1(b) shows the room-temperature PL intensity mapping at 386 nm of the 4H-SiC epilayer. For comparison, the optical microscopy image of the sample surface at the same location is also shown in Fig. 1(c). Note that the region shown in Fig. 1(c) is unusually defective, which was selected to show different defect signals in one PL mapping image. It is evident that more crystalline defect information can be obtained from PL mapping than from optical microscopy. In optical microscopy, only surface morphological defects, such as carrots and comets, can be seen. The other features observed by PL mapping are believed to be the different crystalline defects inside the epilayer, which act as recombination centers. In this letter, we only focus on the planar defects, SFs in the sample, combining PL spectrum and PL intensity mapping to identify their origins and distributions in the sample. SFs in 4H-SiC form quantum-well-like electron states which can be observed by luminescence.¹¹ Due to the

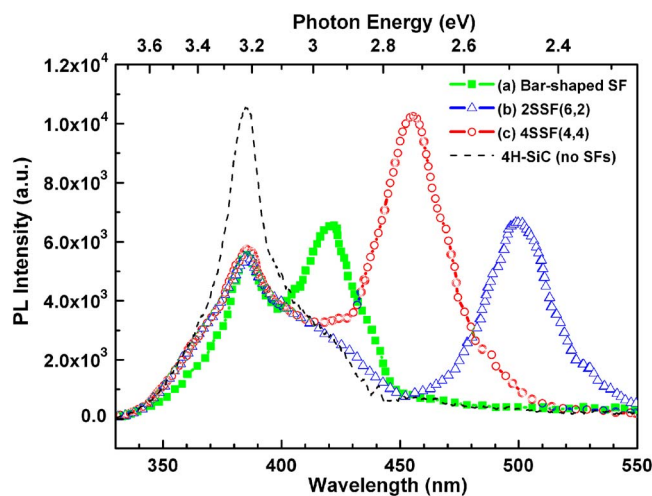


FIG. 2. (Color online) PL spectra from the defective areas: (a) bar-shaped SFs, (b) 2SSFs, and (c) in-grown SFs. (The spectrum from the area without SFs is shown in dashed line).

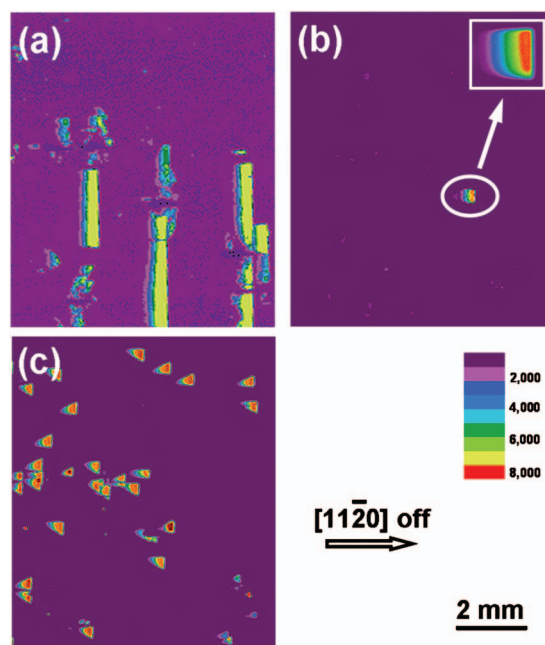


FIG. 3. (Color) PL intensity mapping at (a) 420 nm, (b) 500 nm, and (c) 455 nm.

step-flow epitaxial growth mechanism, the SFs lie in the basal planes. For this reason, the PL signal from the SFs increases in intensity gradually along the step-flow direction from the interface to the surface. The luminescence spectra and the intensity variation are the two main features to characterize the SFs in 4H-SiC epilayers.

The defective areas with bar shapes vertical to the $[11-20]$ direction indicated by A in Fig. 1(b) were characterized. Figure 2(a) shows the PL spectrum obtained from the bar-shaped defect, indicating an additional emission peak at about 420 nm. The PL intensity mapping at 420 nm was performed, as shown in Fig. 3(a). The width of the bars along the step-flow direction $[11-20]$ was approximately $400\text{ }\mu\text{m}$, which corresponds to the projected width of the basal planes in the epilayer ($55\text{ }\mu\text{m}/\tan 8^\circ \approx 400\text{ }\mu\text{m}$). One might conclude that this kind of SF starts at the epilayer/substrate interface only by judging from its width. However, these bar-shaped SFs observed in our sample are not expected to form at the interface, while the SFs expand from the substrate to the epilayer during the epitaxial growth.⁷ The stacking sequence of these bar-shaped SFs are determined to be (5,2) in Zhdanov notation by Hoshino *et al.* using TEM.¹² This means that the bar-shaped SFs are the intrinsic Frank-type SFs (IFSFs). It should be mentioned that the room-temperature PL spectra of the bar-shaped SFs are close to those of the single Shockley SFs (1SSFs) which are observed in degraded *p-i-n* diodes and are generally in the triangular shapes. Although both IFSF and 1SSF show the emission wavelength at approximately 420 nm, the PL spectra of these two kinds of SFs exhibit distinguishable difference in the peak position at low temperature, for example, 4 K.

The area marked by B in Fig. 1(b) exhibits an additional PL peak at around 500 nm, as shown in Fig. 2(b), which is consistent with that reported for double Shockley SF (2SSF).¹³ Figure 3(b) shows the PL intensity mapping at 500 nm. Only one 2SSF was found in this sample. The shape of the 2SSF is close to a rectangle. From a theoretical study, the formation energy of 2SSF in 4H-SiC has been

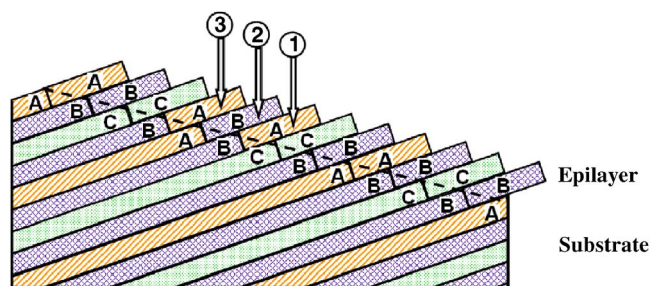


FIG. 4. (Color online) A structural model for the formation of the in-grown SF, 4SSF (4,4), in 4H-SiC.

estimated to be about 21 mJ/m^2 , which is slightly larger than that of the 1SSF ($\sim 18 \text{ mJ/m}^2$).¹⁴ 2SSFs are often reported in heavily nitrogen-doped 4H-SiC annealed at high temperature¹³ or subjected to external mechanical loading.¹⁵ The stacking sequence of 2SSF observed in 4H-SiC is (6,2), like a cubic inclusion embedded in the 4H-SiC.¹⁶ Calculations of the electronic band structure of 4H-SiC in the presence of 2SSF had shown that their electronic properties can be well described by a quantum-well model. The depth of the well of about 0.6 eV is given by the band offset between 4H- and 3C-SiC occurring at the conduction band edge, resulting in the bandgap energy of $\sim 2.6 \text{ eV}$ ($\sim 480 \text{ nm}$) for 2SSF.¹⁷ Considering the redshift of the PL peak from low temperature to room temperature, this value agrees with the position of the room-temperature luminescence band observed from the 2SSF (6,2) in the present sample.

It was found that small distinguished areas marked by C in Fig. 1(b) also emit the additional luminescence besides the band-edge peak, located at 455 nm, as shown in Fig. 2(c). Figure 3(c) shows the PL intensity mapping at 455 nm. The right-angled triangles of the emission areas were clearly identified and composed of the dislocation lines along $[11-20]$ and $[10-10]$ or $[11-20]$ and $[01-10]$. The length of the right-angled triangles along the off-axis direction of $[11-20]$ is approximately $400 \mu\text{m}$, which also corresponds to the projected length of the basal plane in the epitaxial layer. These features make it consistent with the widely reported in-grown SFs in 4H-SiC epilayers.^{18,19} The stacking sequence of the common in-grown SFs in 4H-SiC was confirmed to be 8H (4,4) by different groups, although there might be different SFs which can form during the epitaxial growth. We can expect that 8H (4,4) SFs are formed by four times gliding of Si-C bilayer (BL), for example, gliding two successive BLs and then gliding the followed two successive BLs in the reverse direction, then we can name it as 4SSF (4,4).

As for the real process of the formation of 4SSF (4,4), we can understand it if we look at the step-flow growth process of 4H-SiC. Due to the step-flow growth, the stacking sequences in the epilayer should follow those of the substrate. However, if one BL is faulted in stacking by some extrinsic reasons, for example, the layer of "B" was faulted, as indicated by 1 in Fig. 4, the faulted layer must be converted to A because the underlayer is C. Moreover, its up-layer could not be A anymore and must be changed to B; and

so on, the third faulted layer becomes A, as shown by 3 in Fig. 4. In this case, the fourth layer above it can still follow the stacking sequence of the substrate C. Thus, the 8H (4,4) stacking sequence is locally formed, which is consistent with the TEM results. We checked the PL spectra from more than 60 in-grown SFs and all of the in-grown SFs exhibited the identical PL spectra. This means that all of the in-grown SFs observed in the sample exhibited the identical stacking sequences 4SSF (4,4).

In summary, we have presented micro-PL spectroscopy and PL intensity mapping data characterizing the SFs in 4H-SiC epilayers. SFs with other crystalline defects can be profiled in the PL intensity map performing at the near band edge. To find the details of SFs in the epilayers, its own emission energy was collected first and then PL intensity mapping at this energy was performed. Three kinds of SFs, IFSF (5,2), 2SSF (6,2), and 4SSF (4,4) were identified in our samples. Their shapes and distributions were also determined by PL intensity mapping. Our data lead us to propose that the PL mapping combined with micro-PL spectroscopy can be a practical and effective tool for the nondestructive and rapid characterization of SFs in 4H-SiC wafers.

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